201-14783

HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM

FINAL SUBMISSION

for

TALL OIL FATTY ACIDS AND RELATED SUBSTANCES

CAS No. 61790-12-3
CAS No. 65997-03-7
CAS No. 68955-98-6
CAS No. 68201-37-6
CAS No. 61790-44-1
CAS No. 61790-45-2

Submitted to the US EPA

August 2004

By

The Pine Chemicals Association, Inc.
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HPV Task Force
Consortium Registration

Table of Contents

Final Submission for Tall Oil Fatty Acids and Related Substances

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Summary

As part of the High Production Volume (HPV) Program, the Pine Chemicals Association, Inc. (PCA) has sponsored 6 HPV chemicals. This final summary addresses the following six chemicals, known collectively as Tall Oil Fatty Acids and Tall Oil Fatty Acid Salts:

61790-12-3, Fatty acids, tall-oil
65997-03-7, Fatty acids, tall-oil, low boiling
68955-98-6, Fatty acids, C16-C18 and C18 unsaturated, branched and linear
68201-37-6, Octadecanoic acid, branched and linear
61790-44-1, Fatty acids, tall oil, potassium salts
61790-45-2, Fatty acids, tall oil, sodium salts

This summary encompasses data previously described in the Test Plan for these substances as well as newly acquired data. The totality of the data shows that these chemicals are all non-toxic.

These substances are all derived from or closely related to tall oil fatty acids, a substance obtained by the fractional distillation of crude tall oil, a by-product from the pulping of pine trees. Tall oil fatty acids and their derivatives are all complex mixtures (Class 2 substances) derived from a natural product. Each species of pine tree has a somewhat different mix of fatty acids, and even within a species, the mix of fatty acids could be influenced by the climate and local terrain.

While these are Class 2 substances, all the members of this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts. Thus, PCA elected to treat the group as a category for purposes of the HPV program. Where applicable, PCA conducted physical/chemical property and environmental fate testing on all six substances. However, a representative of the category was used for ecotoxicity and *in vitro* mammalian toxicity testing. Due to the existence of available data on a representative chemical that satisfied the SIDS human health endpoints, no mammalian testing was necessary.

Tall oil fatty acids (CAS# 61790-12-3) ("TOFA") was selected as the representative substance in this group for testing for the additional SIDS ecotoxicity data. This selection was based upon several factors, including the fact that TOFA represents by far the greatest production volume, with almost four times more TOFA manufactured than all other substances in this group combined. In addition, TOFA is the raw material from which all the other group members, except "fatty acids, tall oil, low boiling," are derived. Consequently, test results obtained on TOFA are most representative of the category.

TOFA and the other members of this group are used primarily as raw materials for the production of other chemicals. For example, the largest use of TOFA is in the

production of dimer acids, which are converted into coatings, adhesives and printing inks. TOFA salts are widely used as surfactants in liquid soaps. Other members of the group are used as intermediates in the production of isostearic acid.

The totality of the SIDS data for the substances in this category is briefly summarized below and in Tables 1-3. As shown in these summaries, tall oil fatty acids and related substances are all non-toxic in both mammalian and aquatic test systems. These data are described and discussed in the main document. Detailed Robust Summaries of all relevant data are appended to this document.

Physical/Chemical Properties

The SIDS physical and chemical properties were determined when appropriate; however, many of these endpoints are either inapplicable or cannot be measured for these compounds.

- Melting or boiling points were not determined because these substances will either not give a sharp melting point when heated or will decompose before they melt or boil.
- Under ambient conditions, the vapor pressure of these chemicals is essentially zero and experimental measurement is not possible.
- Water solubility and partition coefficients are summarized in Table 1. It should be noted that although all of the non-salt substances in this category are essentially insoluble in water, considerable effort was undertaken to accurately determine water solubility.
- With respect to the partition coefficient (K_{ow}), the approved method (OECD 117) yields a range of values rather than a single value representative of the mixture. The range of values reflects the partition coefficients of the individual fatty acid constituents of this complex mixture.

The details on these test results are provided in the Robust Summaries.

Table 1. Summary of Physical/Chemical and Environmental Fate Data*

Chemical Name	Required SIDS Endpoint		
	Partition Coefficient	**Water Solubility Mg/l**	**Biodegradation at 28 days**
Fatty acids, tall-oil ("TOFA")	4.9 – 7.6[a]	12.6	56-84%[b]
Fatty acids, tall-oil, low boiling ("heads")	4.4 - 7.8	22.8	41%
Fatty acids, C16-C18 and C18 unsat., branched & linear ("monomer acid")	4.9	15.0	67%
Octadecanoic acid, branched and linear ("hydrogenated monomer acid")	5.6 – 6.1	2.5	46.7%
Fatty acids, tall oil, potassium salts	4.9 – 7.6	Miscible	79%
Fatty acids, tall oil, sodium salts	4.9 – 7.6	Miscible	98.4%

a: A slightly different range was derived from another test; see Robust Summaries for details.
b: These values represent the results from three different tests; see Robust Summaries for details.
*No testing was conducted for melting point, boiling point, vapor pressure, hydrolysis, photodegradation, and transport and distribution between environmental compartments as explained in main document.

Environmental Fate

The SIDS environmental fate endpoints were determined where appropriate; however, many of these endpoints are either inapplicable or cannot be measured for these compounds.

- Photodegradation was not relevant, since the vapor pressure of these compounds is essentially zero and they could not enter the atmosphere.
- Hydrolysis in water was not determined for any of the compounds in this category because all have low water solubility and also lack a functional group that would be susceptible to hydrolysis.
- Transport and distribution between environmental compartments (i.e., fugacity) was not determined due to the inability to provide usable inputs to the required model.
- Biodegradation data are summarized in Table 1 and show that these substances are substantially biodegradable in the environment.

The details on these test results are provided in the Robust Summaries.

Ecotoxicity

TOFA was tested for acute toxicity to fish, daphnia and algae at the maximum measured water solubility. In addition, there are also ecotoxicity data on fatty acids, C16-C18 and C18 unsaturated, branched and linear (i.e., known as monomer acid). These data are summarized in Table 2 and show that none of the compounds in this category are toxic to algae, daphnia or fish. The details of these test results are provided in the Robust Summaries.

Table 2. Summary of Ecotoxicity Data

Chemical Name	Required SIDS Endpoint		
	Acute Fish 96 hr $NOEL_r$	**Acute Daphnia 48 hr $NOEL_r$**	**Acute Algae 72 hr $NOEL_r$**
Fatty acids, tall-oil ("TOFA")	1000 mg/l	1000 mg/l	854 mg/l
Fatty acids, tall-oil, low boiling ("heads")	C	C	C
Fatty acids, C16-C18 and C18 unsat., branched & linear ("monomer acid")	1000 mg/l	1000 mg/l	1000 mg/l
Octadecanoic acid, branched and linear ("hydrogenated monomer acid")	C	C	C
Fatty acids, tall oil, potassium salts	C	C	C
Fatty acids, tall oil, sodium salts	C	C	C

C = Indicates category read-down from available data
$NOEL_{50}$ = no observed effect loading rate

Mammalian Toxicity

For the SIDS human health endpoints, there were sufficient data for TOFA on acute and repeat dose toxicity, *in vitro* genotoxicity in *Salmonella* (i.e., Ames test), and reproductive and developmental effects. TOFA was tested *in vitro* for genotoxicity in a mammalian chromosome aberration test (OECD 473) both with and without metabolic activation. In addition, as described below, there are also acute oral toxicity data on both the sodium and calcium salts of monomer acid, mammalian chromosomal aberration data on monomer acid calcium salt and *in vitro* genotoxicity in *Salmonella* for monomer acid sodium salt. The mammalian toxicity data are summarized in Table 3 and demonstrate that TOFA is non-toxic. Based on the category approach, results for the test substance also represent other members of the category. The details of these test results are provided in the Robust Summaries.

Table 3. Summary of Mammalian Toxicity Data

Chemical Name	Required SIDS Endpoints				
	Acute Oral	**Repeat Dose**	**Genetox (Bacteria)**	**Genetox (Mammalian cells)**	**Repro/ Develop**
Fatty acids, tall-oil ("TOFA")	LD_{50} > 10000 mg/kg	NOEL = 2500 mg/kg/d	+S9 Neg. -S9 Neg.	+S9 -S9 Clastogenic only at overtly toxic concentrations ± S9	No effects; NOEL = 5000 mg/kg/d
Fatty acids, tall-oil, low boiling ("heads")	C	C	C	C	C
Fatty acids, C16-C18 and C18 unsat., branched & linear ("monomer acid")	C	C	C	C	C
Octadecanoic acid, branched and linear ("hydrogenated monomer acid")	C	C	C	C	C
Fatty acids, tall oil, potassium salts	C	C	C	C	C
Fatty acids, tall oil, sodium salts	C	C	C	C	C
Monomer acid, Na salt (not HPV chemical)	LD_{50} > 2500 mg/kg		+S9 Neg. -S9 Neg.		
Monomer acid, Ca salt (not HPV chemical)	LD_{50} > 2500 mg/kg			+S9 Neg. -S9 Neg.	

C= Indicates category read-down from available data.

Non-HPV substances

Overall Hazard Evaluation and Potential Exposure

For potential human health effects, the totality of the SIDS data demonstrates that TOFA is non-toxic. Because all of the chemicals in this group are derived from or closely related to TOFA, as well as the fact that all members of this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts, based on the category approach, it can be inferred that all of the substances in this group are also non-toxic. In addition, the finding of no acute toxicity or *in vitro* genotoxicity for the sodium and calcium salts of monomer acid is further confirmation that the substances in this category are all non-toxic.

TOFA has no acute oral toxicity (i.e., LD_{50} > 10,000 mg/kg), and repeat dose toxicity data demonstrate a no observed effect level (NOEL) of approximately 2500 mg/kg/day. There was no evidence of reproductive or developmental toxicity in a full two-generation study. The lack of acute oral toxicity (i.e., LD_{50} > 2,500 mg/kg) for the sodium and calcium salts of monomer acid is confirmatory of the lack of acute toxicity of the substances in this category. Genotoxicity test results show no evidence of mutagenicity in *Salmonella* (i.e., Ames test) for either TOFA or monomer acid sodium salt. Chromosomal aberrations in Chinese hamster ovary (CHO) cells were evident only at concentrations of TOFA that were overtly toxic to the cells; monomer acid calcium salt was non-clastogenic in human lymphocytes both in the presence and absence of metabolic activation. Consequently, no adverse health consequences would be associated with any exposures to TOFA or related substances. For potential ecotoxicological effects, the data on TOFA and monomer acid demonstrate that all of the substances in this category are non-toxic to aquatic organisms including fish, daphnia and algae.

With respect to potential exposure to the substances in this category, all are consumed almost entirely as industrial intermediates where they are reacted or further distilled to produce other chemicals. Of the various TOFA distillation and reaction products, it is estimated that greater than 75% are marketed and consumed in non-dispersive commercial applications in the production of dimer acids, polyamide adhesive resins, alkyd resins for paint, polyester lubricants, plasticizers, and metal working fluids. Volatization to air and hence inhalation exposure would be minimal due to the essential lack of a vapor pressure for these substances. Exposure in all of these industrial applications is generally limited to dermal contact during manufacture of the numerous products derived from TOFA and related substances.

The Pine Chemicals Association, Inc. HPV Task Force includes the following companies:

Akzo Nobel Resins
Akzo Nobel - Eka Chemicals Incorporated
Arizona Chemical Company
Asphalt Emulsion Manufacturers Association
Boise Cascade Corporation
Cognis Corporation
Crompton Corporation
Eastman Chemical Co. (including the former Hercules Inc. Resins Division)
Georgia-Pacific Resins Inc.
Hercules Incorporated
ICI Americas (including the former Uniqema)
Inland Paperboard & Packaging, Inc.
International Paper Co. (including the former Champion International Corporation)
Koch Materials Co.
McConnaughay Technologies, Inc.
MeadWestvaco (including the former Mead Corp. and the former Westvaco)
Packaging Corporation of America
Plasmine Technology, Inc.
Raisio Chemicals
Rayonier
Riverwood International
Smurfit – Stone Container Corporation
Weyerhaeuser Co.

The Task Force has filed multiple test plans covering various chemicals. Not all members of the Task Force produce the substances covered by this final submission.

Final Submission for Tall Oil Fatty Acids and Related Substances

I. Description of Tall Oil Fatty Acids and Related Substances

The Pine Chemicals Association, Inc. (PCA) sponsored six HPV chemicals known collectively as Tall Oil Fatty Acids and Tall Oil Fatty Acid Salts. The Test Plan for this group of substances was posted on EPA's HPV website on June 14, 2001, with comments from the Physicians Committee for Responsible Medicine (PCRM) and EPA posted on November 1, 2001 and December 3, 2001, respectively. After reviewing these comments, PCA prepared a response (March 3, 2002) which was subsequently posted on EPA's HPV website.

This group of chemicals consists of the following:

61790-12-3, Fatty acids, tall oil
65997-03-7, Fatty acids, tall oil, low boiling
68955-98-6, Fatty acids, C16 - C18 and C18 unsaturated, branched and linear
68201-37-6, Octadecanoic acid, branched and linear
61790-44-1, Fatty acids, tall oil, potassium salts
61790-45-2, Fatty acids, tall oil, sodium salts

All of the chemicals in this group are derived from or closely related to tall oil fatty acids (TOFA), a substance obtained by the fractional distillation of crude tall oil, a by-product from the pulping of pine trees. All the members of this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts. As complex mixtures derived from a natural product, TOFA and its derivatives are all considered Class 2 substances.

Fatty acids are present in the pine tree as glycerol esters and are saponified to sodium salts during the pulping process. These sodium salts are the major component of tall oil soap that is skimmed from spent pulping liquor and acidulated to form crude tall oil. Crude tall oil is then fractionally distilled at high temperatures under vacuum to yield several fractions, two of which are included in this group: TOFA (CAS# 61790-12-3) and fatty acids, tall oil, low boiling (CAS# 65997-03-7). The remaining members of this group are all derived from TOFA (Zinkel and Russell 1989).

A. Composition

Each species of pine tree has a somewhat different mix of fatty acids. Even within a species, the mix of fatty acids may be influenced by the climate and local terrain. Consequently, product specifications for these substances are not given in terms of chemical components, but in general terms such as acid number and iodine value, which are measures of aggregate chemical reactivity (Zinkel and Russell 1989). Provided below is some general information on the typical compositions of each of the six substances in this category.

1. Fatty Acids, Tall Oil (CAS# 61790-12-3)

The composition of a typical tall oil fatty acid (TOFA) is shown in Table 4.

Table 4

Composition of a Typical Tall Oil Fatty Acid

Common Name	***Chemical Structure***	***Percent Composition***
Palmitic acid	$CH_3(CH_2)_{14}COOH$	1
Stearic acid	$CH_3(CH_2)_{16}COOH$	2
Oleic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$	48
Linoleic acid	$CH_3(CH_2)_4CH{=}CH\text{-}CH_2CH{=}CH(CH_2)_7COOH$	35
Conjugated linoleic acid[a]	$CH_3(CH_2)_XCH{=}CHCH{=}CH\text{-}(CH_2)_YCOOH$	7
Other acids[b]		4
Unsaponifiable matter		2

a: x usually 4 or 5; y usually 7 or 8; but x + y = 12

b: 5,9,12-octadecatrienoic acid; linolenic acid; 5,11,14-eicosatrienoic acid; cis,cis-5,9-octadecadienoic acid; eicosadienoic acid; elaidic acid; cis-11 octadecenoic acid; C-20, C-22, C-24 saturated acids.

2. Fatty Acids, Tall Oil, Low Boiling (CAS# 65997-03-7)

The composition of tall oil, low boiling, better known as "tall oil heads," is even more complex. As with TOFA, the composition of heads depends on the origin of the tall oil and the fractionation conditions. The TSCA Inventory defines tall oil heads as, *"the low boiling fraction obtained by the distillation of tall oil. Contains fatty acids such as palmitic, stearic, oleic and linoleic as well as neutral materials."* The neutral component is also complex, and contains small amounts of various terpenic hydrocarbons, alcohols, aldehydes, phenolics, lignin-derived materials, and other neutral materials. The composition of a typical tall oil heads is shown in Table 5.

Table 5

Composition of a Typical Tall Oil Heads

Common Name	*Chemical Structure*	*Percent Composition*
Palmitic acid	$CH_3(CH_2)_{14}COOH$	36
Stearic acid	$CH_3(CH_2)_{16}COOH$	1
Oleic acid	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$	32
Linoleic acid	$CH_3(CH_2)_4CH{=}CH\text{-}CH_2CH{=}CH(CH_2)_7COOH$	23
Other acids[a]		8
Unsaponifiable matter		10

a: These are the same as indicated in Table 2 except the amounts of C20, C22, and C24 will be negligible.

3. Fatty Acids, C16-C18 and C18 Unsaturated, Branched and Linear (CAS# 68955-98-6)

Fatty acids, C16-C18 and C18 unsaturated, branched and linear (CAS# 68955-98-6) is better known as monomer acid. It is a co-product obtained in the production of dimer acid from TOFA. (Dimer acid is sponsored under PCA's Dimers and Trimer Test Plan.) It has some of the characteristics of TOFA, except that it has a much lower level of unsaturation and also contains some branched chains. Monomer acid is a complex mixture of fatty acids; the major components of a typical product are shown in Table 6.

Table 6

Composition of a Typical Monomer Acid

Common Name	*Chemical Structure*	*Percent Composition*
Palmitic acid	$CH_3(CH_2)_{14}COOH$	3
Stearic acid	$CH_3(CH_2)_{16}COOH$	3
Branched C18 acids		28
Oleic acid (cis)	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$	12
Elaidic acid (trans)	$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$	24
Other C18 acids[a]		24
Unsaponifiable matter		1

a: Probably cyclic acids of unknown structure.

4. Octadecanoic Acid, Branched and Linear (CAS# 68201-37-6)

Octadecanoic acid, branched and linear (CAS# 68201-37-6) is also known as hydrogenated monomer acid. It is an intermediate in the conversion of monomer acid into isostearic acid. Its composition is similar to the typical monomer acid shown in Table 6 except that all the acids are saturated.

5. Fatty acids, Tall Oil, Potassium Salt (CAS# 61790-44-1) and Sodium Salt (CAS# 61790-45-2)

Fatty acids, tall oil, potassium salt (CAS# 61790-44-1) and fatty acids, tall oil sodium salt (CAS# 61790-45-2) are simple salts of TOFA. The salts are made by treating TOFA with the appropriate base. As they are salts of a weak acid and a strong base, solutions of these salts are alkaline, with the pH depending on the concentration.

B. Commercial Uses of Tall Oil Fatty Acids and Tall Oil Fatty Acid Salts

Tall oil fatty acids (TOFA) is by far the most important member of this group from a commercial standpoint. The main use of TOFA is as a raw material for the production of a wide variety of other chemicals. TOFA has few, if any, uses in its unmodified form. The largest single use of TOFA is for the production of dimer acids that are then converted into coatings, adhesives, and printing inks. (Dimer acids are addressed in another test plan.) Another important end use for tall oil fatty acids is in the production of alkyd resins that go into paints and printing inks. In all of these applications, TOFA improves the film forming properties and drying characteristics of the products into which it is formulated.

The salts of TOFA are widely used as surfactants. The sodium or potassium salts are used in liquid soaps for both industrial and household cleaning and disinfectant products. They also find uses in metal working fluids and in lubricants.

Tall oil heads are generally consumed for their fuel value. Alternatively, when the fatty acid content is sufficiently high, the heads can be sold for its fatty acid value in some of the same markets that use TOFA.

Monomer acid is used in the production of isostearic acid, a liquid C18 acid. In addition, monomer acid can be used in some of the same applications as TOFA, such as soaps and lubricants.

Octadecanoic acid, branched and linear (hydrogenated monomer) is an intermediate in the production of isostearic acid from monomer acid and does not have any other specific commercial use.

Additional information concerning uses, production and potential exposures to the chemicals in this category are described in greater detail below in the section on *Potential Exposure to Tall Oil Fatty Acids and Related Substances*

C. Complexity of Analytical Methodology

All of the substances in this group are Class 2 substances. This, combined with the fact that fatty acids are essentially insoluble in water and decompose on heating at high temperature, created a variety of analytical challenges. Gas chromatography of methylated derivatives was the method used for the analysis of the members of this category. Because the solubility of the free acids is very low (about 10 ppm), the reliability of this analytical method was verified at such low concentrations.

II. Rationale for Selection of Representative Compound for Testing

TOFA (CAS# 61790-12-3) was selected as the representative substance in this group for testing for the applicable SIDS ecotoxicity and *in vitro* mammalian genotoxicity tests. All the substances in this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts. The selection of TOFA as the representative substance was based on several factors. It has by far the greatest production volume, with almost four times more TOFA manufactured than all other substances in this group combined (i.e., 4, 64, and 28 times greater volume than the low boiling fraction, octadecanoic acid, and fatty acids, C16-18, respectively). EPA guidance suggests that testing the substance produced at the greatest volume as the representative chemical of a category would be appropriate. Clearly, TOFA fits this criterion. In addition, TOFA is the raw material from which all the other group members, except for tall oil heads, are derived.

Another criterion listed by EPA for grouping chemicals into a category is the use of the "family approach" of examining related chemicals when they are acids or acid salts. Although the salts of tall oil fatty acids have quite different physical characteristics, they are included in this group because they are quickly converted into the free acids when they are neutralized by acid or by dilution, as they would be under typical toxicity testing conditions. In summary, this group of chemicals fits the requirements of the EPA's HPV Challenge program for a chemical category, and TOFA is the most appropriate representative test material from this group.

After reviewing the *Test Plan for Tall Oil Fatty Acids and Related Substances*, EPA suggested that PCA form a separate category comprised solely of monomer acid (CAS # 68955-98-6) and octadecanoic acid (CAS # 68201-37-6). The Agency questioned whether the test results for TOFA would be representative of these two members of the category due to the branched and linear nature of these two compounds. After carefully considering these comments, PCA concluded that the category should remain as originally proposed in the test plan. Nonetheless, in light of EPA's comments, the Robust Summaries in this document provide additional data from testing conducted by a PCA member company on monomer acid sodium or calcium salts. Although these chemicals are not HPV chemicals (i.e., not currently on IUR and not assigned CAS Numbers), both of these salts of monomer acid will readily dissociate into monomer acid in aqueous solution; thus, the test results for either of these monomer acid salts should be the functional equivalent of the non-salt (i.e., monomer acid). Likewise, the results should also be representative of octadecanoic acid due to similarity of composition and structure. Octadecanoic acid is simply the hydrogenated form of monomer acid. Moreover, since EPA's HPV Guidelines for grouping chemicals into a category endorses the use of the "family approach" of examining related chemicals when they are acids or acid salts, the use of data on the monomer acid sodium or calcium salts as a surrogate for monomer acid is appropriate. These data are included in the robust summaries.

Finally, EPA also noted that it would be helpful to confirm that the branched and cyclic constituents present in two of the category members arise in the processing of tall oil fatty acids to dimer. Based on our knowledge of the chemistry of the formation of monomer acid, the cyclic structures in monomer are predominantly 1,2-disubstituted six-membered rings that arise from the cyclization of the linoleic and linolenic acids present in TOFA. The formation of cyclic acids in monomer is analogous to the well-documented formation of these same structures in heated vegetable fats such as soybean, linseed, and sunflower oils except that the reaction is acid-catalyzed rather than occurring through a radical mechanism as in the case of heated oils.

III. Summary of Data

At the onset of the HPV program, considerable data were available that satisfied most of the SIDS endpoints for this category. Because there were adequate data for most of the human health SIDS endpoints, no additional testing in mammals was necessary in order to complete the required data for the substances in this category. Table 7 summarizes the results from all of the testing conducted on the substances in this category. Table 7 also illustrates where ecotoxicity data or human health effects data from TOFA, monomer acid, or monomer acid sodium or calcium salts can be generalized to other category members.

Table 7
Summary of Data
Tall Oil Fatty Acids and Related Substances*

Chemical Name and CAS No.	**Key SIDS Endpoints**										
	Partition Coefficient	**Water Sol. Mg/l**	**Biodeg. @ 28 days**	**Acute Fish 96 hr. $NOEL_r$**	**Acute Daph. 48 hr. $NOEL_r$**	**Acute Algae 72hr. $NOEL_r$**	**Acute oral**	**Repeat Dose**	**Genetox *Salmonella***	**Genetox (mammal-ian cells)**	**Repro/ Develop**
Fatty acids, tall-oil 61790-12-3	4.9 – 7.6	12.6	56% 74% 84%	1000 mg/l	1000 mg/l	854 mg/l	LD_{50} > 10,000 mg/kg	NOEL= 2,500 mg/kg/d	Neg. ± S9	Clastogen (± S9) only at overtly toxic conc.	No effects: NOEL> 5,000 mg/kg/d
Fatty acids, tall-oil, low boiling 65997-03-7	4.4 – 7.8	22.8	41%	C	C	C	C	C	C	C	C
Fatty acids, C16-C18 and C18 unsat., branched & linear 68955-98-6	4.9	15.0	67%	1000 mg/l	1000 mg/l	1000 mg/l	C	C	C	C	C
Octadecanoic acid, branched and linear 68201-37-6	5.6 – 6.1	2.5	47%	C	C	C	C	C	C	C	C
Fatty acids, tall oil, potassium salts 61790-44-1	4.9 – 7.6	Miscible	79%	C	C	C	C	C	C	C	C
Fatty acids, tall oil, sodium salts 61790-45-2	4.9 – 7.6	Miscible	98%	C	C	C	C	C	C	C	C
Monomer acid, Sodium salt							LD_{50} > 2,500 mg/kg		Neg. ± S9		
Monomer acid, Calcium salt							LD_{50} > 2,500 mg/kg			Neg. ± S9	

C Indicates category read-down from existing data; *No testing was conducted for melting point, boiling point, vapor pressure, hydrolysis, photodegradation, and transport and distribution between environmental compartments as explained in the summary document.

Monomer acid sodium or calcium salts; not sponsored, non-HPV chemicals; no CAS #'s assigned; testing explained in summary document.

A. Physicochemical Data

The basic physicochemical data required in the SIDS battery includes melting point, boiling point, vapor pressure, partition coefficient (K_{ow}), and water solubility.

Class 2 substances are composed of a complex mixture of substances and are often difficult to characterize. Tall oil fatty acids and their derivatives are Class 2 substances that are derived from natural sources. Their composition is variable and cannot be represented by a definite chemical structural diagram. Due to this "multi-component" characteristic of tall oil fatty acids and their derivatives, some physical property measurements are not appropriate as explained below.

In commenting on the Test Plan for TOFA and related substances, EPA suggested that certain physicochemical properties (i.e., vapor pressure and photodegradation) be measured or estimated for some of the individual components of the complex mixtures that comprise all of the members of this category. PCA disagreed with this suggestion primarily because none of the individual components of these complex mixtures is representative of the mixture itself. Rather, this would provide information on chemicals that were outside of PCA's commitment (i.e., substances with different CAS numbers). However, with respect to this issue, the Soap and Detergent Association has agreed to sponsor chemicals that comprise some of the major constituents of TOFA. Thus, EPA will obtain extensive physicochemical data on some of the components of the complex mixtures in this category.

1. Melting Point

TOFA and the other non-salts in this grouping category are liquids at room temperature. In addition, a sharp melting point cannot be obtained due to the complex nature of these substances. Even though the two salts are solids under ambient conditions, heating them to determine the melting point would cause thermal decomposition. Consequently, the melting point was not determined for any of the substances in this category.

2. Boiling Point

All of the non-salt members of this category are produced by high temperature, high vacuum distillation and are non-volatile at ambient temperatures. A boiling point has no significance because these materials will thermally decompose before they boil, when heated to high temperatures. The two salts in this group are solids. When heated to high temperatures, they will also thermally decompose before boiling. Accordingly, measurement of this property was inappropriate for all the substances in this category.

3. Vapor Pressure

Vapor pressures for the fatty acids at ambient temperatures are effectively zero, and their experimental measurement is inappropriate. The salt members of the group are solids and thus have no vapor pressure, so this end point cannot be measured. When dissolved in water their solutions will reflect the vapor pressure of the water rather than the salt, and therefore measurement of this property is inappropriate.

4. Water Solubility

The water solubility of all six compounds in this category was determined using OECD (105) with the results shown in Table 8.

Table 8

Chemical	Water Solubility (mg/l)
Fatty acids, tall oil	12.6
Fatty acids, tall oil, low boiling	22.8
Fatty acids, C16 - C18 and C18 unsaturated, branched and linear (monomer)	15.0
Octadecanoic acid, branched and linear	2.5
Fatty acids, tall oil, potassium salts	Miscible
Fatty acids, tall oil, sodium salts	Miscible

All of these data are presented in detail in the Robust Summaries.

5. Partition Coefficient

Partition coefficient (i.e., K_{ow}) data were available for TOFA, fatty acids, tall-oil, low boiling, and fatty acids, C16-C18 and C18 unsaturated, branched & linear. Data on K_{ow} were determined for three members of this category - octadecanoic acid, branched and linear; fatty acids, tall oil, potassium salts; and fatty acids, tall oil, sodium salts using OECD (107). Although there were adequate data for TOFA, this substance was retested with the other compounds in this category. Because all of the substances in this category are complex mixtures, the procedure (OECD 117) to determine the K_{ow} yields a range of separate values rather than a single value representative of the mixture reflecting the partition coefficients of the individual fatty acid constituents in this complex mixture. The partition coefficient data are shown in Table 9.

Table 9

Chemical	Partition Coefficient (K_{ow})
Fatty acids, tall oil	4.9 – 7.6
Fatty acids, tall oil, low boiling	4.4 - 7.8
Fatty acids, C16 - C18 and C18 unsaturated, branched and linear (monomer)	4.9
Octadecanoic acid, branched and linear	5.6 – 6.1
Fatty acids, tall oil, potassium salts	4.9 – 7.6
Fatty acids, tall oil, sodium salts	4.9 – 7.6

All of these data are presented in detail in the Robust Summaries.

B. Environmental Fate Data

The fate or behavior of a chemical in the environment is determined by the rates or half-lives for the most important transformation (degradation) processes. The basic environmental fate data covered by the HPV Program includes biodegradation, stability in water (hydrolysis as a function of pH), photodegradation and transport and distribution between environmental compartments.

1. Biodegradation

Biodegradability can help to determine the fate of chemicals in the environment because it provides a measure for the potential of compounds to be degraded by microorganisms. Depending on the nature of the test material, several standard test methods are available to assess potential biodegradability. For the substances in this category OECD method 302B was used for the salts and OECD method 301B was used for the non-salts. Existing and new data were generated using different protocols as noted below.

Of the six chemicals in this category, four (TOFA; tall oil fatty acids, low boiling; fatty acids, C16-C18 and C18 unsaturated, branched and linear; and fatty acids, potassium salts) had existing data on the biodegradation endpoint. Biodegradation for “octadecanoic acid, branched and linear” and “tall oil fatty acids, sodium salts” was determined. The data are summarized below in Table 10.

Table 10

Chemical	Percent Biodegradation	Test Method
Fatty acids, tall oil (Test 1)	56	OECD 301D
Fatty acids, tall oil (Test 2)	84	OECD 301F
Fatty acids, tall oil (Test 3)	74	OPPTS 853.110
Fatty acids, tall oil, low boiling	41	OECD 301D
Fatty acids, C16 - C18 and C18 unsat. branched and linear (monomer)	67	OPPTS 853.110
Octadecanoic acid, branched and linear	47	OECD 301B
Fatty acids, tall oil, potassium salts	79	OPPTS 853.110
Fatty acids, tall oil, sodium salts	98	OECD 302B

All of these data are presented in greater detail in the Robust Summaries.

2. Hydrolysis

Hydrolysis as a function of pH is used to assess the stability of a substance in water. Hydrolysis is a reaction in which a water molecule (or hydroxide ion) substitutes for another atom or group of atoms present in an organic molecule. If there is no group suitable to be displaced, then the organic compound is considered to be resistant to hydrolysis. None of the substances in the tall oil fatty acids category contains an organic functional group that might be susceptible to this physical degradative mechanism. Therefore, hydrolysis was not measured for any of the substances in this category.

In addition, low water solubility often limits the ability to determine hydrolysis as a function of pH. All of the tall oil fatty acids have very low solubility in water. Therefore, these materials are expected to be stable in water and it would be unnecessary to attempt to measure the products of hydrolysis. With respect to the fatty acid salts, since they exist in an aqueous medium they hydrolyze (ionize) immediately, but form stable species. Consequently, it was also unnecessary to measure this endpoint for the fatty acid salts.

3. Photodegradation

Due to their low water solubility and lack of any vapor pressure, there is no opportunity for any of the substances in this category to enter the atmosphere. Thus, photodegradation is irrelevant. In addition, based on the constituents in these complex mixtures, there is no reason to suspect that they would be subject to breakdown by a photodegradative mechanism. Consequently, this endpoint was not be determined for any of the substances in this category.

4. Transport and Distribution between Environmental Compartments

The transport and distribution between environmental compartments (i.e., fugacity) is intended to determine the ability of a chemical to move or partition in the environment. There are various mathematical models for estimating fugacity. One of the most frequently referenced models is the level III model from the Canadian Environment Modeling Centre at Trent University. Even the simplest of these models requires estimates of solubility, vapor pressure and octanol/water partition coefficient to estimate fugacity for a single component. For complex class 2 substances such as TOFA and related substances, estimates of any one of these physical parameters for the various known components would span a range of more that a order of magnitude. When combining three or more parameters of equally variable ranges to derive estimates for different environmental media, the variability in the estimate for any given medium would grow geometrically to more that three or more orders of magnitude. This suggests that any estimates based on arbitrarily selected individual components would be essentially useless for any practical purpose. Add to this the additional fact that there is variability in the chemical composition of these substances (as illustrated in Tables 4, 5 and 6, above) and the possible permutations become unmanageable. Consequently, for complex mixtures such as TOFA and related substances, the mathematical models which rely upon estimates for individual components are of no practical use in predicting environmental fate. Consequently, due to the inability to provide usable inputs to the required model, no determination of transportation and distribution between environmental compartments was undertaken for tall oil fatty acids and related compounds

C. Ecotoxicity Data

The basic ecotoxicity data that are part of the HPV Program include acute toxicity to fish, daphnia and algae. While there were existing data on these endpoints for some of the substances in this category, these data were conflicting and it was difficult to determine which, if any, of these findings is representative of true ecotoxicity. The inconsistencies in how water samples were prepared for testing these endpoints rendered these data inadequate. Consequently, acute toxicity to fish, daphnia and alga was retested for TOFA under the same conditions that were used to measure the limit of water solubility. In addition, these tests were conducted under conditions that were designed to maximize the solubility under the specific test exposure conditions, but reduce exposure to insoluble fractions, which may cause nonspecific toxicological effects. In addition, the effect of both filtering, to further minimize nonspecific physical effects, and of reducing the pH to the lower end of the acceptable range for test organism survival, was also investigated for changes in toxicological effects. The results of preliminary tests were used to select the most appropriate test conditions for the definitive test for each species.

In reviewing the *Test Plan for TOFA and Related Substances*, EPA agreed with the proposed acute toxicity testing of fish, daphnia, and algae, but also suggested that PCA conduct a 21-day chronic daphnid reproduction test using a flow-through method with measured concentrations. A 21-day test using a flow-through method would be impracticable, based on the amount of water that would be required due to the substances' extremely low solubility and the difficulty in performing the necessary serial analytical measurements. In addition, where there is a risk of emulsions forming inherently (as there is likely to be with these substances), flow through testing in not possible and is not recommended in OECD (2000) Guidance Document 23 (Aquatic Toxicity Testing of Difficult Substances and Mixtures). As noted above, the methodology for preparing the water for ecotoxicity testing was identical to that used to determine the solubility of TOFA. This procedure was adopted in order to ensure that ecotoxicity testing was conducted at the limit of actual water solubility.

Finally, both EPA and OECD guidance recommend the use of 21-day testing only if the substances have the potential for long-term effects in the aquatic environment, i.e., are bioaccumulative -- which these substances are not. The high K_{ow} values for the components of TOFA (i.e., individual fatty acids) reflect the fact that they are lipid-like materials and not that they bioaccumulate. Thus, chronic aquatic toxicity testing in daphnia should not be necessary for the HPV Program.

It should also be noted that in accordance with EPA's suggestion that the data on TOFA might not be representative of fatty acids, C16 - C18 and C18 unsaturated, branched and linear (i.e., monomer acid) or octadecanoic acid, branched and linear, included in the robust summaries are ecotoxicity data (i.e., fish, daphnia and algae) for monomer acid as well as recently developed ecotoxicity data (i.e., fish and daphnia) on monomer acid, calcium salt. The ecotoxicity data are summarized below in Table 11 and demonstrate that both TOFA and monomer acid are non-toxic to fish, daphnia and algae.

Table 11

Chemical	**Fish 96 hr. *$NOEL_r$**	**Daphnia 48 hr. $NOEL_r$**	**Algae 72 hr. $NOEL_r$**
Fatty acids, tall oil	1000 mg/l	1000 mg/l	500 mg/l
Monomer acid[a]	1000 mg/l	1000 mg/l	1000 mg/l
Monomer acid, calcium salt[b]	100 mg/l	100 mg/l	

*$NOEL_r$ = No Observed Effect Loading Rate
a = For monomer acid all effects were reported as no observed effect concentration loading rates ($LOEC_r$)
b= Highest loading rate tested

These data are presented in greater detail in the Robust Summaries.

D. Human Health Effects Data

1. Acute Oral Toxicity

Acute oral toxicity studies investigate the effect(s) of a single exposure to a relatively high dose of a substance. This test is conducted by administering the test material to animals (typically rats or mice) in a single gavage dose. Harmonized EPA testing guidelines (August 1998) set the limit dose for acute oral toxicity studies at 2000 mg/kg body weight. If less than 50 percent mortality is observed at the limit dose, no further testing is needed. A test substance that shows no effects at the limit dose is considered nontoxic. If compound-related mortality is observed, then further testing may be necessary.

Summary of Acute Oral Toxicity Data

TOFA is non-toxic following acute oral exposure. TOFA was tested for acute oral toxicity in Sprague-Dawley rats. Animals received a single oral (gavage) dose of 10,000 mg/kg and were observed for 14 days. Parameters evaluated included clinical signs, mortality, body weight, and gross pathology. None of the animals died. One hour post-dosing, piloerection was observed in one male and abnormal stance was observed in one male and one female. By four hours, these effects had resolved. No body weight effects were observed. Gross necropsy revealed no treatment-related effects. The acute oral LD_{50} was >10,000 mg/kg. Similarly, both the sodium and calcium salts of monomer acid are non-toxic following acute oral exposure with the oral LD_{50}'s for both > 2500 mg/kg. These data are presented in greater detail in the Robust Summaries.

2. Repeat Dose Toxicity

Subchronic repeated dose toxicity studies are designed to evaluate the effect of repeated exposure to a chemical over a significant period of the life span of an animal. Typically, the exposure regimen in a subchronic study involves daily exposure (at least 5 consecutive days per week) for a period of not less than 28 days or up to 90 days (i.e., 4 to 13 weeks). The HPV program calls for a repeat dose test of at least 28 days. The dose levels evaluated are lower than the relatively high limit doses used in acute toxicity (i.e., LD_{50}) studies. In general, repeat dose studies are designed to assess systemic toxicity, but the study protocol can be modified to incorporate evaluation of potential adverse reproductive and/or developmental effects.

Summary of Repeat Dose Toxicity Data

There are substantial data that demonstrate a lack of toxicity for TOFA. Tall oil fatty acid (CAS #61790-12-3) was tested in a 90-day subchronic toxicity study in rats. The test material was administered to Charles River rats in the diet at concentrations 0, 5, 10, or 25% for 90 days. The approximate doses were 0, 2500, 5000, or 12,500 mg/kg/day. Parameters evaluated included clinical signs, mortality, body weight, body weight gain, food consumption, hematology, clinical chemistry, urinalysis, gross pathology, organ weights, and microscopic pathology.

There were no deaths attributable to the test compound and no clinical signs were observed. Body weight and body weight gain were not affected by treatment, but food consumption was slightly decreased at dietary levels of 10 and 25%. No changes in hematology, clinical chemistry or urinalysis parameters were measured at any dose level. At gross pathology, no treatment-related effects were noted. No consistent organ weight changes and no histopathological effects were reported. Based on these data, the No Observed Effect Level (NOEL) was 5% (approximately 2500 mg/kg/day). Other subchronic studies for 28 and 40 days confirm the low toxicity of TOFA. In these studies, the only effect noted was depression of body weight gain at the highest doses tested. These data are presented in greater detail in the Robust Summaries.

3. Genotoxicity – In vitro

Genetic testing is conducted to determine the effects of substances on genetic material (i.e., DNA and chromosomes). Genetic mutations are commonly measured in bacterial and mammalian cells, and the HPV program calls for completing both types of tests. The genotoxicity data are summarized below in Table 12 and show that TOFA and monomer acid, sodium salt are negative in the Ames *Salmonella* test, monomer acid, calcium is non-clastogenic in mammalian cells while TOFA was clastogenic only at concentrations that were overtly toxic to the cells.

Table 12

Chemical	Ames *Salmonella* +S9	Ames *Salmonella* -S9	Chromosomal Aberration +S9	Chromosomal Aberration -S9
TOFA	Neg.	Neg.	Clastogenic (at overtly toxic concentration)	Clastogenic (at overtly toxic concentration)
Monomer acid Sodium salt	Neg.	Neg.		
Monomer acid Calcium salt			Non-clastogenic	Non-clastogenic

These data are presented in greater detail in the Robust Summaries.

4. Reproductive and Developmental Toxicity

Reproductive toxicity includes any adverse effect on fertility and reproduction, including effects on gonadal function, mating behavior, conception, and parturition. Developmental toxicity is any adverse effect induced during the period of fetal development, including structural abnormalities, altered growth and post-partum development of the offspring.

Summary of Reproductive/Developmental Toxicity Data

TOFA had no effects when tested for reproductive and developmental toxicity in Sprague-Dawley rats in a full two-generation study. The test compound was administered in the diet at concentrations of 0, 5 or 10% to 30 females/group and 15 males/group. The approximate doses were 0, 2500, or 5000 mg/kg/day. Males and females in the first generation (F_0) began treatment at 80 days of age and were mated at 100 days of age. Treatment of the F_0 animals continued through the weaning of the first generation (F_1). After weaning, the F_1 males and females were maintained on the treatment diet. At 100 days of age, they were mated and allowed to deliver pups (F_2).

There were no treatment-related effects on reproductive performance, or on any parameter measured in either the F_1 or F_2 pups. No treatment-related changes in fertility, viability, lactation, or gestation indices were observed. Hematology, clinical chemistry and urinalysis parameters were similarly unchanged, and there were no developmental effects in any F_1 or F_2 offspring. TOFA did not alter or otherwise affect the reproduction or development of rats in this study at doses as high as 10% (approximately 5000 mg/kg/day). These data are presented in greater detail in the Robust Summaries.

IV. Category Justification: Validation of Tall Oil Fatty Acids as Representative of Other Category Members for SIDS Endpoints

All of the substances in this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts. In addition, except for tall oil heads, TOFA is the raw material from which all the other group members are derived. However, even for tall oil heads, the composition is qualitatively similar to other members in this category. For TOFA (including sodium and potassium salts) and tall oil heads the primary difference in their respective composition is in the ratios of palmitic, stearic, oleic, linoleic acid, other C18 acids and unsaponifiable matter. On the other hand, monomer acid contains branched and linear constituents including unsaturated oleic acid (cis) and elaidic acid (trans) which are both substantially saturated in hydrogenated monomer. Because the totality of the toxicity data for TOFA demonstrates that it is non-toxic, it is reasonable to infer that the TOFA salts and tall oil heads are similarly non-toxic. While it is also reasonable to conclude that monomer acid and hydrogenated monomer (octadecanoic acid) are similarly non-toxic, additional data add further to this likelihood.

Acute toxicity and *in vitro* mutagenicity data on monomer acid sodium or calcium salts were also available. It is well known that both of these salts of monomer acid will readily dissociate into monomer acid in aqueous solution. Thus, the finding of no acute toxicity or *in vitro* mutagenicity for either salt test is the functional equivalent of the non-salt (i.e., monomer acid). These results are also representative of octadecanoic acid due to similarity of composition and structure since octadecanoic acid is simply the hydrogenated form of monomer acid. In addition, acute ecotoxicity data were also available for monomer acid and monomer acid, calcium salt which demonstrate that neither substance was acutely toxic to fish, daphnia or algae. In summary, based on adequate toxicity data and a detailed understanding of the composition of the six substances in this category, the toxicological data on TOFA (augmented by data on monomer acid and monomer acid salts) can be reliably extrapolated to the entire category thereby validating the composition of the category.

V. Hazard Characterization of Tall Oil Fatty Acids and Related Substances

For potential human health effects, the totality of the SIDS data demonstrates that TOFA is non-toxic. Because all of the chemicals in this group are derived from or closely related to TOFA, as well as the fact that all members of this group are similar in chemical composition, being predominantly C18 unsaturated and saturated fatty acids, or their salts, based on the category approach, it can be inferred that all of the substances in this group are also non-toxic. In addition, the finding of no acute toxicity or *in vitro* genotoxicity for the sodium and calcium salts of monomer acid is further confirmation that the substances in this category are all non-toxic.

TOFA has no acute oral toxicity (i.e., LD_{50} > 10,000 mg/kg), and repeat dose toxicity data demonstrate a no observed effect level (NOEL) of approximately 2500 mg/kg/day. There was no evidence of reproductive or developmental toxicity in a full two-generation study. The lack of acute oral toxicity (i.e., LD_{50} > 2,500 mg/kg) for the sodium and calcium salts of monomer acid is confirmatory of the lack of acute toxicity of the substances in this category. Genotoxicity test results show no evidence of mutagenicity in *Salmonella* (i.e., Ames test) for either TOFA or monomer acid sodium salt. Chromosomal aberrations in Chinese hamster ovary (CHO) cells were evident only at concentrations of TOFA that were overtly toxic to the cells while monomer acid calcium salt was non-clastogenic in human lymphocytes both in the presence and absence of metabolic activation. Consequently, no adverse health consequences would be associated with any anticipated exposures to TOFA or related substances.

With respect to potential ecotoxicological effects, the totality of SIDS data on TOFA, the representative substance in this category, as well as for monomer acid, and monomer acid, calcium salt demonstrate that the substances in this category are non-toxic to aquatic organisms including fish, daphnia and algae. The No Observed Effect Loading Rate ($NOEL_r$) for TOFA to both fish and daphnia was 1000 mg/l while the $NOEL_r$ for algae was 500 mg/l. For monomer acid, the no observed effect concentration loading rate ($NOEC_r$) was 1000 mg/l in fish, daphnia and algae. Finally, for monomer acid, calcium salt the $NOEL_r$ for both fish and daphnia was 100 mg/l (i.e., the highest loading rate tested).

VI. Potential Exposure to Tall Oil Fatty Acids and Related Substances

This brief summary provides an overview of market end uses and potential exposure to products derived from Tall Oil, a major feed stock to the pine chemicals industry with emphasis on tall oil fatty acids and related substances. This information along with hazard data developed as part of the High Production Volume Chemical Testing Program should be useful in evaluating the potential risks (if any) that might be associated with various uses of tall oil derived chemicals.

During the process of pulping coniferous trees to make paper, sodium salts of chemicals occurring naturally in the trees are produced as a co-product. When acidulated, this soap becomes Tall Oil. Typically, Tall Oil is a mixture of 25–35% rosin acids and 45–55% fatty acids with the balance being neutral compounds. Tall oil can be further processed or separated into its major components by a process of high temperature low pressure distillation. The recovery and distillation of tall oil began on a commercial scale in the mid twentieth century. As the pulp and paper industry has expanded globally so has the processing of tall oil, and the production of tall oil derivatives. At the present time there are 10 companies operating a total of 19 tall oil distillation plants in 10 countries. The total production of tall oil is approximately two billion pounds per year.

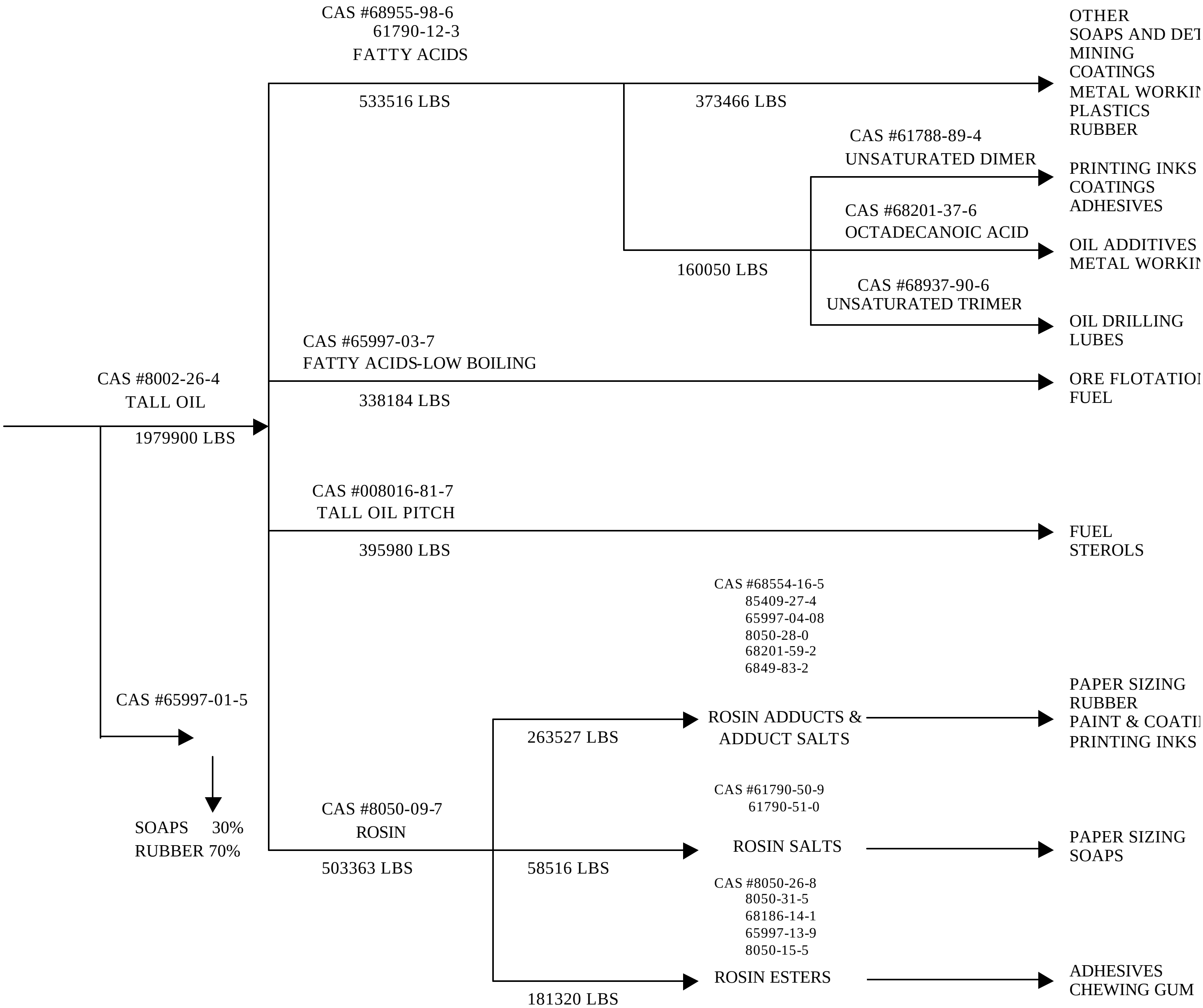
Human exposure is limited by the fact that most tall oil chemicals are industrial intermediates consumed in the production of other chemicals As such there is little, if any, potential for exposure of the general consumer population. Environmental exposure is limited by the fact that the chemical processes used in the tall oil industry are essentially closed system processes where temperature and pressure are carefully controlled.

Environmental releases from tall oil processing plants are limited to (1) treated waste water discharge, and (2) ambient emissions following treatment with scrubbers or thermal oxidizers. Waste water can be generated from operation of the plant pressure control system or from minor spills and leaks associated with the process and/or handling of chemical products and routine housekeeping activities. In all cases the waste water is collected, the stream is treated to remove any free oil, and is then discharged into a lager biological waste treatment facility (either municipal treatment system or the treatment system of the parent company's paper mill). Air emissions generated from the pressure control system or from the storage and transfer of various streams, are generally collected and treated in chemical scrubbers or thermal oxidizers.

The entire array of tall oil based chemicals and their related processing steps are best depicted by a "family tree" or flow diagram rather than a listing of discrete independent chemicals. Such a diagram demonstrates how various "parent" chemicals are consumed in the production of down stream chemicals. Figure 1 is a representation of the "family tree" for tall oil products and the relationship between

U.S. TALL OIL INDUSTRY

PRODUCTION & MARKET DISTRIBUTION
POUNDS/YEAR (000)



these products. Based on industry data approximately 95% of tall oil is consumed during the production of other downstream products.

Two primary fractions (rosin, fatty acids) are derived form the initial processing of tall oil. As can be seen from Figure 1 these primary fractions are further processed to a wide variety of intermediates. Tall oil “Heads,” tall oil “Pitch” and distilled tall oil (DTO) are the remaining fractions derived from the processing of tall oil. Each of these fractions or intermediates and their end uses are described in the appropriate Post-testing Final Summary documents for each category of substances.

Tall Oil Fatty Acids & Salts

Tall oil fatty acids (TOFA) are consumed almost entirely as an industrial intermediate where they are reacted or further distilled to produce other chemicals. Table 13 illustrates general use categories and potential exposures to TOFA and related substances. Of the various TOFA distillation and reaction products, it is estimated that greater than 75% are marketed and consumed in non-dispersive commercial applications in the production of dimer acids, polyamide adhesive resins, alkyd resins for paint, polyester lubricants, plasticizers, and metal working fluids. Volatization to air and hence inhalation exposure would be minimal due to the essential lack of a vapor pressure for these substances. Exposure in all of these industrial applications is generally limited to dermal contact during manufacture of the numerous products derived from TOFA and related substances.

Approximately 12% of TOFA production is marketed into the soap and detergent industry. In this application TOFA is reacted to form salts which are constituents in these consumer products. In addition, a small percentage of TOFA production is further processed into oleic and linoleic acids which are cleared for use as direct food additives by the US FDA. The only other potential exposure to any of the substances in this category occurs during their production from activities such as changing reaction vessels, sampling for quality control, transferring material from one work area to another, loading and unloading bulk containers, changing filters, and cleaning equipment.

Table 13

Distribution, Application and Potential Occupational Exposure to Fatty Acids and Related Substances

Substance	CAS #	Primary Function	Use Category	Major End Use Application	%
Fatty Acids, Tall Oil Fatty Acid, C-16,-C18 and C18 unsaturated, branched and linear (monomer acid)*	61790-12-3 68955-98-6	Chemical intermediate (feed for fatty acid derivatives)	Site limited/ Industrial	Salts Mining Paints & coatings Plastics Dimer Other	31 17 11 7 30 4
Fatty Acids, Low Boiling	65997-03-7	Chemical intermediate	Industrial	Mining Fuel	90 10
Octadecanoic Acid, Branched & Linear	68201-37-6	Chemical intermediate (feed for iso-stearic acid)	Site limited/ industrial	Oil additives Metal working	85 15
Fatty acids, tall oil, potassium salt Fatty acids, tall oil, sodium salt	61790-44-1 61790-45-2	Chemical intermediate (surfactants)	Site limited/ industrial	Soaps Metal working fluids Lubricants	61 29 10

*Addressed in Final Submission for Fatty Acid Dimers and Trimer

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August 2004